



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 03:38 am BST

PDB ID : 6N0N  
Title : Crystal structure of Tdp1 catalytic domain in complex with compound XZ574  
Authors : Lountos, G.T.; Zhao, X.Z.; Kiselev, E.; Tropea, J.E.; Needle, D.; Burke Jr., T.R.; Pommier, Y.; Waugh, D.S.  
Deposited on : 2018-11-07  
Resolution : 1.48 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

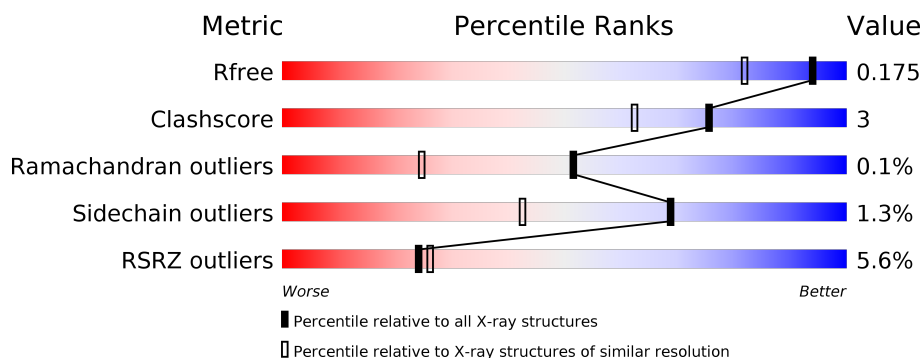
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.48 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4690 (1.50-1.46)
Clashscore	141614	4955 (1.50-1.46)
Ramachandran outliers	138981	4846 (1.50-1.46)
Sidechain outliers	138945	4844 (1.50-1.46)
RSRZ outliers	127900	4614 (1.50-1.46)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	461	<div> <div>7%</div> <div> <div></div> <div>87%</div> <div>8%</div> <div>5%</div> </div> </div>
1	B	461	<div> <div>3%</div> <div> <div></div> <div>86%</div> <div>8%</div> <div>5%</div> </div> </div>

## 2 Entry composition [i](#)

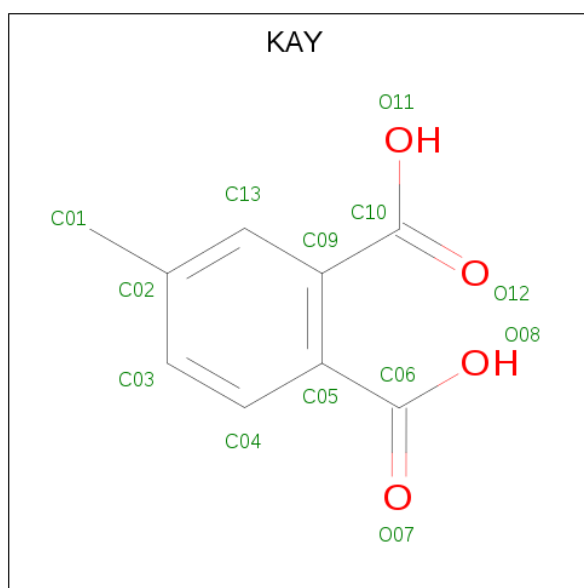
There are 5 unique types of molecules in this entry. The entry contains 8189 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Tyrosyl-DNA phosphodiesterase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	0	18	0
			3632	2351	614	652	15			
1	B	437	Total	C	N	O	S	0	18	0
			3634	2350	614	656	14			

- Molecule 2 is 4-methylbenzene-1,2-dicarboxylic acid (three-letter code: KAY) (formula:  $C_9H_8O_4$ ).



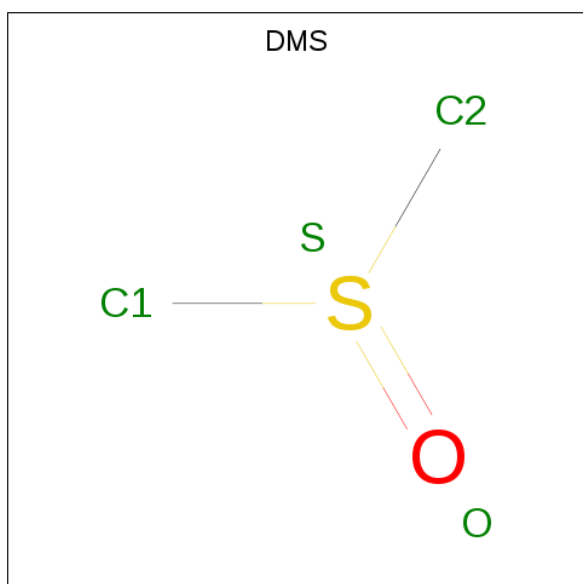
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	9	4		
2	B	1	Total	C	O	0	0
			13	9	4		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula:  $C_2H_6OS$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 4	C 2	O 1	S 1	0	0
4	B	1	Total 4	C 2	O 1	S 1	0	0

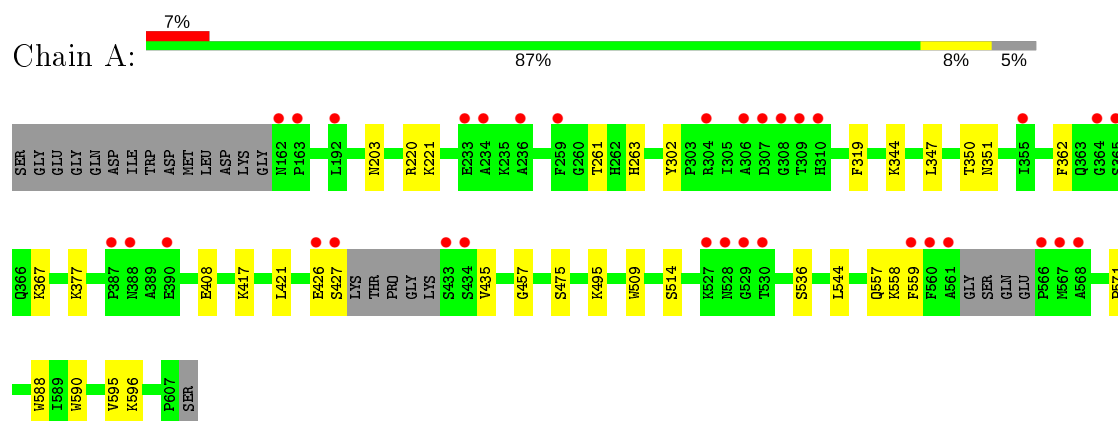
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	394	Total 394	O 394	0	0
5	B	475	Total 475	O 475	0	0

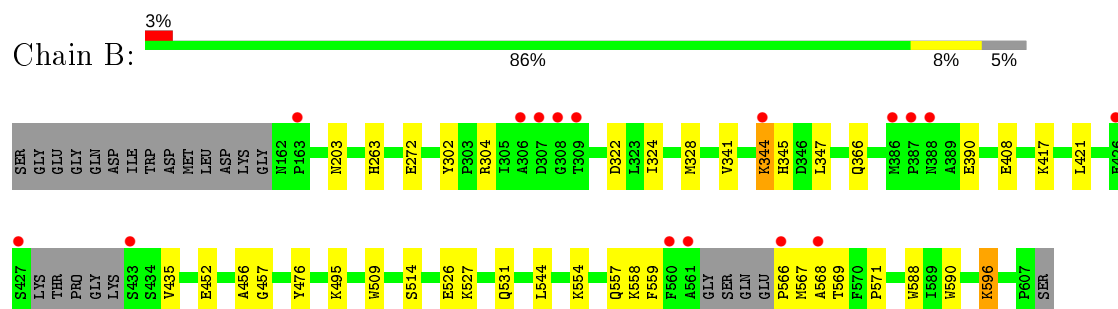
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Tyrosyl-DNA phosphodiesterase 1



#### • Molecule 1: Tyrosyl-DNA phosphodiesterase 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	49.93Å 105.20Å 193.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.98 – 1.48 36.98 – 1.48	Depositor EDS
% Data completeness (in resolution range)	99.5 (36.98-1.48) 95.5 (36.98-1.48)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.85 (at 1.48Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, $R_{free}$	0.163 , 0.175 0.163 , 0.175	Depositor DCC
$R_{free}$ test set	2000 reflections (1.17%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.4	Xtriage
Anisotropy	0.436	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 50.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	8189	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.27% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: KAY, DMS, EDO

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.33	0/3750	0.55	0/5093
1	B	0.42	1/3752 (0.0%)	0.58	0/5098
All	All	0.38	1/7502 (0.0%)	0.56	0/10191

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	344	LYS	CE-NZ	-14.62	1.12	1.49

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3632	0	3548	19	0
1	B	3634	0	3537	25	0
2	A	13	0	0	0	0
2	B	13	0	0	0	0
3	A	8	0	12	0	0
3	B	12	0	18	2	0
4	A	4	0	6	0	0
4	B	4	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	394	0	0	6	0
5	B	475	0	0	6	0
All	All	8189	0	7127	45	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (45) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:LYS:NZ	5:A:801:HOH:O	2.11	0.83
1:B:322:ASP:HB3	3:B:703:EDO:H21	1.66	0.77
1:B:554:LYS:NZ	5:B:802:HOH:O	2.24	0.68
1:B:304:ARG:HE	1:B:344:LYS:HE3	1.60	0.67
1:A:595:VAL:HG23	1:A:596:LYS:HE2	1.83	0.61
1:B:324:ILE:O	1:B:328[B]:MET:HG3	2.02	0.60
1:B:566:PRO:O	1:B:568:ALA:N	2.34	0.59
1:B:526[B]:GLU:OE2	1:B:531:GLN:NE2	2.34	0.58
1:A:408:GLU:OE1	5:A:802:HOH:O	2.17	0.58
1:A:417:LYS:O	1:A:421[A]:LEU:HG	2.04	0.58
3:B:703:EDO:H22	5:B:1007:HOH:O	2.05	0.56
1:B:417:LYS:O	1:B:421[A]:LEU:HG	2.06	0.55
1:B:272:GLU:OE2	5:B:801:HOH:O	2.18	0.55
1:B:557:GLN:NE2	5:B:806:HOH:O	2.39	0.53
1:A:421[A]:LEU:HD22	1:A:435:VAL:HG11	1.90	0.52
1:B:408:GLU:OE1	1:B:476:TYR:OH	2.24	0.52
1:B:557:GLN:C	1:B:558:LYS:HD2	2.31	0.51
1:B:421[A]:LEU:HD22	1:B:435:VAL:HG11	1.92	0.50
1:B:390:GLU:CD	1:B:390:GLU:H	2.15	0.50
1:A:509:TRP:HB3	1:A:544:LEU:HD23	1.94	0.50
1:B:366:GLN:NE2	5:B:814:HOH:O	2.44	0.50
1:B:341:VAL:O	1:B:344:LYS:HG2	2.13	0.48
1:B:596:LYS:HD3	5:B:1037:HOH:O	2.13	0.47
1:B:457:GLY:HA3	1:B:588:TRP:CZ2	2.50	0.46
1:B:344:LYS:HE2	1:B:345:HIS:HE1	1.79	0.46
1:B:302:TYR:CD1	1:B:347:LEU:HA	2.51	0.46
1:A:457:GLY:HA3	1:A:588:TRP:CZ2	2.51	0.46
1:B:559:PHE:CE2	1:B:571:PRO:HB2	2.51	0.46
1:B:452:GLU:HB2	1:B:456:ALA:HB2	1.98	0.45
1:B:527:LYS:NZ	1:B:531:GLN:HE22	2.14	0.45
1:A:377:LYS:NZ	5:A:811:HOH:O	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:TYR:CD1	1:A:347:LEU:HA	2.53	0.43
1:A:319:PHE:CG	1:A:350:THR:HG21	2.53	0.43
1:B:566:PRO:O	1:B:569:THR:HG23	2.17	0.43
1:A:351[B]:ASN:ND2	5:A:815:HOH:O	2.51	0.43
1:A:557:GLN:O	1:A:558:LYS:HD3	2.19	0.43
1:A:261:THR:O	1:A:536[A]:SER:OG	2.23	0.42
1:A:427:SER:O	5:A:803:HOH:O	2.22	0.42
1:A:426:GLU:OE1	1:A:426:GLU:N	2.52	0.42
1:B:263[B]:HIS:CE1	1:B:514:SER:O	2.73	0.42
1:A:362:PHE:O	1:A:367:LYS:HG2	2.21	0.41
1:B:509:TRP:HB3	1:B:544:LEU:HD23	2.02	0.41
1:A:263[B]:HIS:CE1	1:A:514:SER:O	2.74	0.40
1:A:263[A]:HIS:HE1	5:A:1136:HOH:O	2.04	0.40
1:A:559:PHE:CE2	1:A:571:PRO:HB2	2.56	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	449/461 (97%)	441 (98%)	8 (2%)	0	100	100
1	B	449/461 (97%)	440 (98%)	8 (2%)	1 (0%)	47	23
All	All	898/922 (97%)	881 (98%)	16 (2%)	1 (0%)	51	25

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	567	MET

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	397/400 (99%)	390 (98%)	7 (2%)	59	29
1	B	397/400 (99%)	393 (99%)	4 (1%)	76	54
All	All	794/800 (99%)	783 (99%)	11 (1%)	69	40

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	203	ASN
1	A	220	ARG
1	A	221	LYS
1	A	475[A]	SER
1	A	475[B]	SER
1	A	495	LYS
1	A	590	TRP
1	B	203	ASN
1	B	495	LYS
1	B	590	TRP
1	B	596	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	310	HIS
1	B	237	HIS
1	B	366	GLN
1	B	531	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

9 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	EDO	B	704	-	3,3,3	0.43	0	2,2,2	0.33	0
2	KAY	B	701	-	9,13,13	2.62	2 (22%)	9,18,18	1.16	0
2	KAY	A	701	-	9,13,13	2.75	2 (22%)	9,18,18	1.17	0
4	DMS	B	705	-	3,3,3	0.66	0	3,3,3	0.69	0
3	EDO	A	703	-	3,3,3	0.48	0	2,2,2	0.25	0
4	DMS	A	704	-	3,3,3	0.60	0	3,3,3	0.51	0
3	EDO	B	702	-	3,3,3	0.56	0	2,2,2	0.20	0
3	EDO	A	702	-	3,3,3	0.48	0	2,2,2	0.35	0
3	EDO	B	703	-	3,3,3	0.40	0	2,2,2	0.32	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	B	704	-	-	0/1/1/1	-
2	KAY	B	701	-	-	0/0/8/8	0/1/1/1
2	KAY	A	701	-	-	0/0/8/8	0/1/1/1
3	EDO	A	703	-	-	0/1/1/1	-
3	EDO	B	702	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	702	-	-	0/1/1/1	-
3	EDO	B	703	-	-	1/1/1/1	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	KAY	C05-C06	5.92	1.53	1.47
2	B	701	KAY	C05-C06	5.85	1.53	1.47
2	A	701	KAY	C09-C10	5.53	1.52	1.47
2	B	701	KAY	C09-C10	4.87	1.52	1.47

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	703	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	703	EDO	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	437/461 (94%)	0.13	33 (7%) 13 15	15, 26, 49, 72	0
1	B	437/461 (94%)	-0.04	16 (3%) 41 45	12, 21, 44, 69	0
All	All	874/922 (94%)	0.05	49 (5%) 24 26	12, 23, 48, 72	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	566	PRO	7.3
1	B	566	PRO	6.3
1	A	560	PHE	6.1
1	A	427	SER	5.8
1	B	427	SER	5.5
1	A	308	GLY	5.4
1	A	567	MET	5.1
1	A	163	PRO	4.9
1	A	561	ALA	4.8
1	A	528	ASN	4.4
1	B	307	ASP	4.1
1	B	387	PRO	4.1
1	A	307	ASP	4.0
1	A	387	PRO	3.8
1	A	559	PHE	3.7
1	A	530	THR	3.6
1	B	568	ALA	3.5
1	A	426	GLU	3.5
1	A	433	SER	3.5
1	A	434	SER	3.5
1	A	162	ASN	3.4
1	A	365	SER	3.4
1	B	426	GLU	3.4
1	B	308	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	364	GLY	3.3
1	A	568	ALA	3.3
1	B	163	PRO	3.3
1	A	306	ALA	3.2
1	B	561	ALA	3.1
1	A	259	PHE	3.1
1	A	309	THR	3.1
1	B	309	THR	2.9
1	A	233	GLU	2.9
1	A	388	ASN	2.8
1	B	388	ASN	2.8
1	B	306	ALA	2.7
1	A	236	ALA	2.7
1	B	560	PHE	2.7
1	A	310	HIS	2.6
1	A	390	GLU	2.5
1	A	304	ARG	2.4
1	A	234	ALA	2.4
1	A	527	LYS	2.3
1	A	355	ILE	2.3
1	A	192	LEU	2.2
1	B	344	LYS	2.2
1	B	433	SER	2.1
1	A	529	GLY	2.1
1	B	386	MET	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	EDO	A	703	4/4	0.73	0.30	44,53,60,61	0
4	DMS	B	705	4/4	0.82	0.13	46,55,62,63	0
4	DMS	A	704	4/4	0.86	0.17	55,56,57,57	0
3	EDO	B	703	4/4	0.88	0.24	34,37,40,45	0
3	EDO	B	704	4/4	0.92	0.18	34,41,49,57	0
2	KAY	B	701	13/13	0.97	0.06	15,19,24,30	0
3	EDO	B	702	4/4	0.97	0.09	16,17,20,22	0
3	EDO	A	702	4/4	0.97	0.10	19,19,20,26	0
2	KAY	A	701	13/13	0.97	0.09	18,21,31,34	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.